

Spectral problems about many-body Dirac operators mentioned by Dereziński

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Abstract

We consider spectral problems for many-body Dirac operators mentioned by Dereziński in the IAMP News Bulletin of January 2012. In particular, we derive a representation of the Dirac Coulomb operator for a helium-like ion as a matrix operator of order sixteen. We show that it is essentially self-adjoint (under natural restrictions on the coupling constants), that the essential spectrum of its closure is the whole real line and that it has no eigenvalues.

1 Introduction

In [2], Dereziński mentioned open problems about many-body Dirac operators. These problems were originally formulated by B. Jeziorski who is a chemist from the University of Warsaw (cf. J. Sucher [10] p.6). Among them there are spectral problems on Dirac-Coulomb operator H_{DC} for a helium-like ion, which has the form

$$H_{DC} = H(1, Z) + H(2, Z) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (1.1)$$

where

$$H(i, Z) = c\vec{\alpha}\vec{p}_i + mc^2\beta - \frac{Z}{|\mathbf{r}_i|}, \quad i = 1, 2 \quad (1.2)$$

is the usual Dirac operator for an electron i in the hydrogen-like ion of charge Z and of mass m . In the above notation, \mathbf{r}_i and \vec{p}_i , $i = 1, 2$ are a position vector and the momentum operator, respectively, of the i -th electron,

$$\mathbf{r} = (x_1, x_2, x_3), \quad \vec{p} = -i\hbar \text{grad}.$$

The vector $\vec{\alpha}$ is a vector operator whose components $\alpha_1, \alpha_2, \alpha_3$, together with the operator $\beta \equiv \alpha_4$ are Hermitian matrices of order four satisfying the anti-commuting relations

$$\alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk} \quad (j, k = 1, 2, 3, 4).$$

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Since the domain of the Dirac operator $H(i, Z)$ is a subspace of four-component wave functions depending on the three coordinates of the i -th electron, we may infer that H_{DC} acts on sixteen-component wave functions which depend on the six coordinates of two electrons and have the anti-symmetric property due to the Pauli principle.

Mathematically, the operator should be written as

$$H_{DC} = H(Z) \otimes I + I \otimes H(Z) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (1.3)$$

where

$$H(Z) = c\vec{\alpha} \cdot \vec{p} + mc^2\beta - \frac{Z}{|\mathbf{r}|} \quad (1.4)$$

is an operator in $\mathcal{H} = L^2(\mathbf{R}^3; \mathbf{C}^4)$. The domain of H_{DC} is a subspace of the antisymmetric tensor product $\mathcal{H} \otimes_A \mathcal{H}$.

In this paper we shall rigorously derive a representation of H_{DC} as a matrix operator of order sixteen and give an answer to its spectral problems, especially essential self-adjointness, continuous (essential) spectrum and absence of eigenvalues. Our method was inspired by a simpler model operator (see (4.5)).

2 Two-electron problems

As far as we know, there is no systematic derivation of relativistic systems in the physics and quantum chemistry literature, so that two-body relativistic systems with which we are concerned seem to be less familiar than nonrelativistic ones. The first relativistic equation for two particles which was extensively used in the past was the Breit equation; it is a differential equation for a relativistic wave function for two electrons, interacting with each other and with an external electromagnetic field. It is not fully Lorentz invariant and is only an approximation. It reads (see [1])

$$\left(E - H[1] - H[2] - \frac{e^2}{r_{12}} \right) U = -\frac{e^2}{2r_{12}} \left[\vec{\alpha}_1 \cdot \vec{\alpha}_2 + \frac{(\vec{\alpha}_1 \cdot \mathbf{r}_{12})(\vec{\alpha}_2 \cdot \mathbf{r}_{12})}{r_{12}^2} \right] U, \quad (2.1)$$

where $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$, $r_{12} = |\mathbf{r}_{12}|$ and

$$H[\mathbf{j}] = -e\varphi(\mathbf{r}_j) + \beta_j mc^2 + \vec{\alpha}_j \cdot (c\mathbf{p}_j + e\mathbf{A}(\mathbf{r}_j)) \quad (2.2)$$

is the Dirac Hamiltonian and the Dirac matrices $\vec{\alpha}_j$ and β_j operate on the spinor of U (for electron j). The wave function U depends on the positions \mathbf{r}_1 and \mathbf{r}_2 and has sixteen spinor components.

If we neglect the right hand side of the equation (2.1) with $\mathbf{A} = 0$, then we get the Dirac-Coulomb equation

$$\left(E - H_D[1] - H_D[2] - \frac{e^2}{r_{12}} \right) \Psi = 0, \quad (2.3)$$

where $H_D[\mathbf{j}]$ is the usual Dirac operator acting on the j -th electron:

$$H_D\Psi = \begin{pmatrix} (m+V)I_2 & \vec{\sigma} \cdot \vec{p} \\ \vec{\sigma} \cdot \vec{p} & -(m-V)I_2 \end{pmatrix} \begin{pmatrix} \Psi^\ell \\ \Psi^s \end{pmatrix}, \text{ with } V = -\frac{Z}{|\mathbf{r}|}. \quad (2.4)$$

Here, $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and

$$\vec{\sigma} \cdot \vec{p} = \sum_{i=1}^3 \sigma_i p_i.$$

The letters ℓ and s refer to the large and the small part of the wave function.

In the relativistic theory, we have to handle a two-fold tensor product space of \mathbf{C}^4 -valued functions because the usual Dirac operator acts on four-vectors belonging to $L^2(\mathbf{R}^3; \mathbf{C}^4)$. For $\mathcal{H} = L^2(\mathbf{R}^3; \mathbf{C}^4)$, the two-fold tensor product $\mathcal{H}^{\otimes 2} = \mathcal{H} \otimes \mathcal{H}$ can be identified with

$$\mathcal{H} \otimes \mathcal{H} = \left\{ \psi(\mathbf{1}, \mathbf{2}) = {}^t(\vec{\psi}_{\ell\ell}, \vec{\psi}_{\ell s}, \vec{\psi}_{s\ell}, \vec{\psi}_{ss}) \in L^2(\mathbf{R}^6; \mathbf{C}^{16}) \mid \vec{\psi}_{ij} \in L^2(\mathbf{R}^6; \mathbf{C}^4) \right\}.$$

Here we have identified $L^2(\mathbf{R}^6; \mathbf{C}^4)$ with $L^2(\mathbf{R}^6; \mathbf{C}^2) \otimes \mathbf{C}^2$ in the following way.

For $k = 1, 2$, let

$$L^2(\mathbf{R}^3; \mathbf{C}^4) \ni \psi(\mathbf{k}) = \begin{pmatrix} \psi_1^\ell(\mathbf{r}_k) \\ \psi_2^\ell(\mathbf{r}_k) \\ \psi_1^s(\mathbf{r}_k) \\ \psi_2^s(\mathbf{r}_k) \end{pmatrix} = \left(\psi_1^\ell e_1 + \psi_2^\ell e_2 \right) \otimes f_\ell + \left(\psi_1^s e_1 + \psi_2^s e_2 \right) \otimes f_s,$$

where

$$e_1 = {}^t(1, 0), \quad e_2 = {}^t(0, 1), \quad f_\ell = {}^t(1, 0), \quad f_s = {}^t(0, 1).$$

In this notation, we see that any product function

$$\psi(\mathbf{1}) \otimes \psi(\mathbf{2}) = \sum_{a,b \in \{\ell, s\}} \sum_{i=1}^2 \sum_{j=1}^2 \psi_{a,b,i,j}(\mathbf{r}_1, \mathbf{r}_2) (e_i \otimes e_j) \otimes (f_a \otimes f_b) \quad (2.5)$$

satisfies

$$\vec{\psi}_{ab}(\mathbf{r}_1, \mathbf{r}_2) = \begin{pmatrix} \psi_{a,b,1,1}(\mathbf{r}_1, \mathbf{r}_2) \\ \psi_{a,b,1,2}(\mathbf{r}_1, \mathbf{r}_2) \\ \psi_{a,b,2,1}(\mathbf{r}_1, \mathbf{r}_2) \\ \psi_{a,b,2,2}(\mathbf{r}_1, \mathbf{r}_2) \end{pmatrix} = \begin{pmatrix} \psi_1^a(\mathbf{r}_1) \\ \psi_2^a(\mathbf{r}_1) \end{pmatrix} \otimes \begin{pmatrix} \psi_1^b(\mathbf{r}_2) \\ \psi_2^b(\mathbf{r}_2) \end{pmatrix} = \begin{pmatrix} \psi_1^a(\mathbf{r}_1) \psi_1^b(\mathbf{r}_2) \\ \psi_1^a(\mathbf{r}_1) \psi_2^b(\mathbf{r}_2) \\ \psi_2^a(\mathbf{r}_1) \psi_1^b(\mathbf{r}_2) \\ \psi_2^a(\mathbf{r}_1) \psi_2^b(\mathbf{r}_2) \end{pmatrix}$$

for any $a, b \in \{\ell, s\}$.

Now we shall define two subspaces of $\mathcal{H}^{\otimes 2} = \mathcal{H} \otimes \mathcal{H}$, the anti-symmetric space and symmetric space, denoted by $\mathcal{H}_A^2 = \mathcal{H} \otimes_A \mathcal{H}$ and $\mathcal{H}_S^2 = \mathcal{H} \otimes_S \mathcal{H}$, respectively.

Definition 2.1

$$\begin{aligned} \mathcal{H}_A^2 = & \left\{ \psi(\mathbf{r}_1, \mathbf{r}_2) = {}^t(\vec{\psi}_{11}, \vec{\psi}_{12}, \vec{\psi}_{21}, \vec{\psi}_{22}) \in L^2(\mathbf{R}^6; \mathbf{C}^{16}) \mid \vec{\psi}_{ij} \in L^2(\mathbf{R}^6; \mathbf{C}^4), \right. \\ & \psi_{ij} = \text{Mat}[\vec{\psi}_{ij}] \in L^2(\mathbf{R}^6; M(2, \mathbf{C})), \quad \psi_{k,k}(\mathbf{r}_2, \mathbf{r}_1) = -\psi_{k,k}(\mathbf{r}_1, \mathbf{r}_2), \quad k = 1, 2, \\ & \left. \psi_{1,2}(\mathbf{r}_2, \mathbf{r}_1) = -\psi_{2,1}(\mathbf{r}_1, \mathbf{r}_2) \right\}, \end{aligned}$$

where

$$\text{Mat}[\vec{a}] = \begin{pmatrix} a_1 & a_3 \\ a_2 & a_4 \end{pmatrix} \text{ for } \vec{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} \in \mathbf{C}^4 \quad (2.6)$$

and tM stands for the transposed matrix of the 2×2 matrix M .

Remark 2.1 The definition 2.1 coincides with the one in the literature on quantum chemistry ([6], [7]), where a slightly different notation from ours is adopted.

$$\Psi(\mathbf{1}, \mathbf{2}) = \begin{pmatrix} \vec{\Psi}^{\ell\ell}(\mathbf{1}, \mathbf{2}) \\ \vec{\Psi}^{\ell s}(\mathbf{1}, \mathbf{2}) \\ \vec{\Psi}^{s\ell}(\mathbf{1}, \mathbf{2}) \\ \vec{\Psi}^{ss}(\mathbf{1}, \mathbf{2}) \end{pmatrix} \text{ with } \begin{cases} \vec{\Psi}^{\ell\ell}(\mathbf{1}, \mathbf{2}) = -\vec{\Psi}^{\ell\ell}(\mathbf{2}, \mathbf{1}) \\ \vec{\Psi}^{\ell s}(\mathbf{1}, \mathbf{2}) = -\vec{\Psi}^{s\ell}(\mathbf{2}, \mathbf{1}) \\ \vec{\Psi}^{s\ell}(\mathbf{1}, \mathbf{2}) = -\vec{\Psi}^{ss}(\mathbf{2}, \mathbf{1}) \end{cases} \quad (2.7)$$

Moreover, it should be pointed out that the four components $\vec{\Psi}^{\ell\ell}$, $\vec{\Psi}^{\ell s}$, $\vec{\Psi}^{s\ell}$, $\vec{\Psi}^{ss}$ in (2.7) are not functions from $\mathbf{R}^3 \otimes \mathbf{R}^3$ to \mathbf{C}^4 , but they are functions from $(\mathbf{R}^3 \times \{\uparrow, \downarrow\}) \otimes (\mathbf{R}^3 \times \{\uparrow, \downarrow\})$ to \mathbf{C} .

In a similar way, we can define the symmetric tensor product space.

Definition 2.2

$$\begin{aligned} \mathcal{H}_S^2 = & \left\{ \psi(\mathbf{r}_1, \mathbf{r}_2) = {}^t(\vec{\psi}_{11}, \vec{\psi}_{12}, \vec{\psi}_{21}, \vec{\psi}_{22}) \in L^2(\mathbf{R}^6; \mathbf{C}^{16}) \mid \vec{\psi}_{ij} \in L^2(\mathbf{R}^6; \mathbf{C}^4), \right. \\ & \psi_{ij} = \text{Mat}[\vec{\psi}_{ij}] \in L^2(\mathbf{R}^6; M(2, \mathbf{C})), \psi_{k,k}(\mathbf{r}_2, \mathbf{r}_1) = {}^t\psi_{1,1}(\mathbf{r}_1, \mathbf{r}_2), \quad k = 1, 2, \\ & \left. \psi_{1,2}(\mathbf{r}_2, \mathbf{r}_1) = {}^t\psi_{2,1}(\mathbf{r}_1, \mathbf{r}_2) \right\}. \end{aligned}$$

In the matrix formulation, we define the standard inner product of \mathcal{H}_A^2 or \mathcal{H}_S^2 by

$$\langle \vec{F}, \vec{G} \rangle = \sum_{i,j=1}^2 \int_{\mathbf{R}^6} \text{tr}(F_{ij}(\mathbf{r}_1, \mathbf{r}_2) \overline{{}^tG_{ij}(\mathbf{r}_1, \mathbf{r}_2)}) d\mathbf{r}_1 d\mathbf{r}_2. \quad (2.8)$$

The notation $\langle \vec{F}_{ij}, \vec{G}_{ij} \rangle$ will be used as an abbreviation for the integral over the trace.

3 The two-electron Dirac-Coulomb Hamiltonian

As usual, the free and the one-particle Dirac operator are denoted by

$$H_0 = \vec{\alpha} \cdot \vec{p} + m\beta, \quad H = H_0 + \frac{k}{|\mathbf{r}|} I_4. \quad (3.1)$$

Here $\vec{p} = {}^t(p_1, p_2, p_3)$, $p_j = -i\partial_{\mathbf{r}_j}$; m is a nonnegative number and $k \in \mathbf{R}$.

Theorem 3.2 prepares for a representation of

$$H_{DC} = H_D \otimes I_4 + I_4 \otimes H_D + V_0(\mathbf{r}_1, \mathbf{r}_2), \quad V_0(\mathbf{r}_1, \mathbf{r}_2) = k_0/|\mathbf{r}_1 - \mathbf{r}_2| I_{16} \quad (3.2)$$

in the subspace \mathcal{H}_A^2 of $\mathcal{H}^{\otimes 2} = \mathcal{H} \otimes \mathcal{H}$ which coincides with that used in literature on quantum chemistry ([4], [5], [6]).

Lemma 3.1 *Let*

$$M_j = \begin{pmatrix} B & A_j \\ A_j & -B \end{pmatrix} \in M(2, \mathbf{C}), \quad j = 1, 2. \quad (3.3)$$

Then it holds that

$$M_1 \otimes I_2 + I_2 \otimes M_2 = \begin{pmatrix} 2B & A_2 & A_1 & 0 \\ A_2 & 0 & 0 & A_1 \\ A_1 & 0 & 0 & A_2 \\ 0 & A_1 & A_2 & -2B \end{pmatrix}. \quad (3.4)$$

Proof: In general, the Kronecker product of two matrices $X = (x_{ij})$ and $Y = (y_{ij})$ is defined by

$$X \otimes Y = (x_{ij}Y), \quad (3.5)$$

so that $X \otimes Y$ is a matrix of size $mn \times k\ell$ if X and Y are $m \times n$ and $k \times \ell$ type, respectively.

$$M_1 \otimes I_2 = \begin{pmatrix} B & 0 & A_1 & 0 \\ 0 & B & 0 & A_1 \\ A_1 & 0 & -B & 0 \\ 0 & A_1 & 0 & -B \end{pmatrix}, \quad I_2 \otimes M_2 = \begin{pmatrix} B & A_2 & 0 & 0 \\ A_2 & -B & 0 & 0 \\ 0 & 0 & B & A_2 \\ 0 & 0 & A_2 & -B \end{pmatrix}. \quad (3.6)$$

Q.E.D.

Theorem 3.2 *Let $\mathcal{H}^{\otimes 2} \ni \psi = {}^t(\vec{\psi}_{11}, \vec{\psi}_{12}, \vec{\psi}_{21}, \vec{\psi}_{22}) \in L^2(\mathbf{R}^6; \mathbf{C}^4)$. Then it holds that*

$$(H_0 \otimes I_4 + I_4 \otimes H_0)\psi = \begin{pmatrix} 2mI_4 & h_2 & h_1 & 0 \\ h_2 & 0 & 0 & h_1 \\ h_1 & 0 & 0 & h_2 \\ 0 & h_1 & h_2 & -2mI_4 \end{pmatrix} \begin{pmatrix} \vec{\psi}_{11} \\ \vec{\psi}_{12} \\ \vec{\psi}_{21} \\ \vec{\psi}_{22} \end{pmatrix}, \quad (3.7)$$

where

$$h_1 = (\vec{\sigma} \cdot \vec{p}_1) \otimes I_2, \quad h_2 = I_2 \otimes (\vec{\sigma} \cdot \vec{p}_2). \quad (3.8)$$

Proof: Denote f_ℓ and f_s by \mathbf{i} and \mathbf{j} , respectively. Let us consider two elements of $\mathcal{H}^{\otimes 2}$

$$\Psi = \Psi_1(\mathbf{r}) \otimes \mathbf{i} + \Psi_2(\mathbf{r}) \otimes \mathbf{j}, \quad \Psi' = \Psi'_1(\mathbf{r}) \otimes \mathbf{i} + \Psi'_2(\mathbf{r}) \otimes \mathbf{j}, \quad (3.9)$$

where for $k = 1, 2$,

$$\Psi_k(\mathbf{r}) = \begin{pmatrix} \psi_{k1}(\mathbf{r}) \\ \psi_{k2}(\mathbf{r}) \end{pmatrix}, \quad \Psi'_k(\mathbf{r}) = \begin{pmatrix} \psi'_{k1}(\mathbf{r}) \\ \psi'_{k2}(\mathbf{r}) \end{pmatrix}. \quad (3.10)$$

We can regard Ψ_k ($k = 1, 2$) as functions of $\mathbf{x} = (\mathbf{r}, \omega)$ as follows.

$$\Psi_k(\mathbf{r}, \omega) = \psi_{k1}(\mathbf{r})\chi_+(\omega) + \psi_{k2}(\mathbf{r})\chi_-(\omega), \quad (3.11)$$

where χ_{\pm} are two orthonormal functions describing the spin of electrons.

Then we have

$$\Psi \otimes \Psi' = \Psi_1 \otimes \Psi'_1 \otimes (\mathbf{i} \otimes \mathbf{i}) + \Psi_1 \otimes \Psi'_2 \otimes (\mathbf{i} \otimes \mathbf{j}) + \Psi_2 \otimes \Psi'_1 \otimes (\mathbf{j} \otimes \mathbf{i}) + \Psi_2 \otimes \Psi'_2 \otimes (\mathbf{j} \otimes \mathbf{j}), \quad (3.12)$$

where

$$\Psi_k \otimes \Psi'_\ell = \begin{pmatrix} \psi_{k1}(\mathbf{r}_1)\psi'_{\ell 1}(\mathbf{r}_2) \\ \psi_{k1}(\mathbf{r}_1)\psi'_{\ell 2}(\mathbf{r}_2) \\ \psi_{k2}(\mathbf{r}_1)\psi'_{\ell 1}(\mathbf{r}_2) \\ \psi_{k2}(\mathbf{r}_1)\psi'_{\ell 2}(\mathbf{r}_2) \end{pmatrix} \cong \begin{pmatrix} \psi_{k1}(\mathbf{r}_1)\psi'_{\ell 1}(\mathbf{r}_2) & \psi_{k2}(\mathbf{r}_1)\psi'_{\ell 1}(\mathbf{r}_2) \\ \psi_{k1}(\mathbf{r}_1)\psi'_{\ell 2}(\mathbf{r}_2) & \psi_{k2}(\mathbf{r}_1)\psi'_{\ell 2}(\mathbf{r}_2) \end{pmatrix}. \quad (3.13)$$

We see that

$$\begin{aligned} (H_0 \otimes I_4)(\Psi \otimes \Psi') &= (H_0 \Psi) \otimes \Psi' \\ &= \{(\vec{\sigma} \cdot \vec{p} \Psi_2 + mI_2 \Psi_1)\mathbf{i} + (\vec{\sigma} \cdot \vec{p} \Psi_1 - mI_2 \Psi_2)\mathbf{j}\} \otimes (\Psi'_1 \mathbf{i} + \Psi'_2 \mathbf{j}) \\ &= [(\vec{\sigma} \cdot \vec{p} \Psi_2 + mI_2 \Psi_1) \otimes \Psi'_1] \otimes (\mathbf{i} \otimes \mathbf{i}) + [(\vec{\sigma} \cdot \vec{p} \Psi_2 + mI_2 \Psi_1) \otimes \Psi'_2] \otimes (\mathbf{i} \otimes \mathbf{j}) \\ &\quad + [(\vec{\sigma} \cdot \vec{p} \Psi_1 - mI_2 \Psi_2) \otimes \Psi'_1] \otimes (\mathbf{j} \otimes \mathbf{i}) + [(\vec{\sigma} \cdot \vec{p} \Psi_1 - mI_2 \Psi_2) \otimes \Psi'_2] \otimes (\mathbf{j} \otimes \mathbf{j}). \end{aligned} \quad (3.14)$$

Since the four vectors $\mathbf{i} \otimes \mathbf{i}$, $\mathbf{i} \otimes \mathbf{j}$, $\mathbf{j} \otimes \mathbf{i}$, $\mathbf{j} \otimes \mathbf{j}$ are linearly independent in $\mathcal{H}^{\otimes 2}$, we find

$$\begin{aligned} (H_0 \otimes I_4)(\Psi \otimes \Psi') &= \begin{pmatrix} (\vec{\sigma} \cdot \vec{p} \Psi_2 + mI_2 \Psi_1) \otimes \Psi'_1 \\ (\vec{\sigma} \cdot \vec{p} \Psi_2 + mI_2 \Psi_1) \otimes \Psi'_2 \\ (\vec{\sigma} \cdot \vec{p} \Psi_1 - mI_2 \Psi_2) \otimes \Psi'_1 \\ (\vec{\sigma} \cdot \vec{p} \Psi_1 - mI_2 \Psi_2) \otimes \Psi'_2 \end{pmatrix} \\ &= \begin{pmatrix} mI_4 & 0 & (\vec{\sigma} \cdot \vec{p}) \otimes I_2 & 0 \\ 0 & mI_4 & 0 & (\vec{\sigma} \cdot \vec{p}) \otimes I_2 \\ (\vec{\sigma} \cdot \vec{p}) \otimes I_2 & 0 & -mI_4 & 0 \\ 0 & (\vec{\sigma} \cdot \vec{p}) \otimes I_2 & 0 & -mI_4 \end{pmatrix} \begin{pmatrix} \Psi_1 \otimes \Psi'_1 \\ \Psi_1 \otimes \Psi'_2 \\ \Psi_2 \otimes \Psi'_1 \\ \Psi_2 \otimes \Psi'_2 \end{pmatrix}. \end{aligned} \quad (3.15)$$

Similarly, the identity

$$(I_4 \otimes H_0)(\Psi \otimes \Psi') = \Psi \otimes (H_0 \Psi') = (\Psi_1 \mathbf{i} + \Psi_2 \mathbf{j}) \otimes \{(\vec{\sigma} \cdot \vec{p} \Psi'_2 + mI_2 \Psi'_1)\mathbf{i} + (\vec{\sigma} \cdot \vec{p} \Psi'_1 - mI_2 \Psi'_2)\mathbf{j}\} \quad (3.16)$$

implies

$$\begin{aligned} (I_4 \otimes H_0)(\Psi \otimes \Psi') &= \begin{pmatrix} mI_4 & I_2 \otimes (\vec{\sigma} \cdot \vec{p}) & 0 & 0 \\ I_2 \otimes (\vec{\sigma} \cdot \vec{p}) & -mI_4 & 0 & 0 \\ 0 & 0 & mI_4 & I_2 \otimes (\vec{\sigma} \cdot \vec{p}) \\ 0 & 0 & I_2 \otimes (\vec{\sigma} \cdot \vec{p}) & -mI_4 \end{pmatrix} \begin{pmatrix} \Psi_1 \otimes \Psi'_1 \\ \Psi_1 \otimes \Psi'_2 \\ \Psi_2 \otimes \Psi'_1 \\ \Psi_2 \otimes \Psi'_2 \end{pmatrix}. \end{aligned} \quad (3.17)$$

Q.E.D.

4 Main results

The following spectral properties of the usual Dirac operator

$$H = \vec{\alpha} \cdot \vec{p} + m\beta - k/|\mathbf{r}|I_4 \quad (4.1)$$

with $m > 0$ are well-known (see, e.g., [11], [14]).

1. H is essentially selfadjoint on $C_0^\infty(\mathbf{R}^3)^4$ if $|k| \leq \sqrt{3}/2$.
2. $\sigma_{\text{ess}}(H) = \mathbf{R} \setminus (-m, m)$ if $|k| \leq \sqrt{3}/2$.
3. If $|k| \leq \sqrt{3}/2$, then H has no eigenvalues in $\mathbf{R} \setminus (-m, m)$ and there are countably many eigenvalues in $(-m, m)$ whose only accumulating points are $\pm m$.

When the scalar potential $k/|\mathbf{r}|$ is replaced by any symmetric matrix potential $V(\mathbf{r})$ satisfying $|V(\mathbf{r})| \leq k/|\mathbf{r}|$, we have

4. $\vec{\alpha} \cdot \vec{p} + m\beta + V(\mathbf{r})$ is essentially selfadjoint on $C_0^\infty(\mathbf{R}^3)^4$ if $|k| < 1/2$.

Now we shall state our main results for the Hamiltonian

$$H_{DC} = H \otimes I_4 + I_4 \otimes H + \frac{k_0}{|\mathbf{r}_1 - \mathbf{r}_2|} I_{16}. \quad (4.2)$$

These are just the first attempts to answer the spectral problem.

Theorem 4.1 *Suppose that $|k| < \sqrt{3}/2$. Then, for any nonzero real k_0 , H_{DC} is essentially selfadjoint on $[C_0^\infty(\mathbf{R}^3; \mathbf{C}^4)]^{\otimes 2} \cap \mathcal{H}_A^2$.*

Remark 4.1 *The same conclusion is true if we replace the Coulomb potentials $k/|\mathbf{r}_j|$ by any symmetric matrix potentials $V(\mathbf{r}_j)$ satisfying*

$$|V(\mathbf{r}_j)| \leq k'/|\mathbf{r}_j|, \quad j = 1, 2. \quad (4.3)$$

with $|k'| < 1/2$.

The unique self-adjoint extension is denoted by the same symbol H_{DC} again.

Theorem 4.2 *Suppose that $|k| < \sqrt{3}/2$. Then, for any nonzero real k_0 , we have*

$$\sigma_{\text{ess}}(H_{DC}|_{\mathcal{H}_A^2}) = \mathbf{R}. \quad (4.4)$$

Theorem 4.3 *Suppose that $|k| < \sqrt{3}/2$. Then, for any nonzero real k_0 , $H_{DC}|_{\mathcal{H}_A^2}$ has no eigenvalues.*

We also consider the following simple model operator \mathbb{H}

$$\mathbb{H} := \alpha p_1 + \alpha p_2 + 2m\beta + \frac{k_1}{|\mathbf{r}_1|} + \frac{k_2}{|\mathbf{r}_2|} + \frac{k_0}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (4.5)$$

in $L^2(\mathbf{R}^6)^4$. It is easier to handle than H_{DC} because an orthogonal change of variables reduces it to a Dirac operator in $L^2(\mathbf{R}^3)^4$ with a double-well potential.

Theorem 4.4 *If $|k_j| < \sqrt{3}/2$ ($j = 1, 2$), \mathbb{H} on $C_0^\infty(\mathbf{R}^6)^4$ is essentially self-adjoint for any $k_0 \in \mathbf{R}$.*

Let \mathbb{H} denote the unique self-adjoint extension again.

Theorem 4.5 *Suppose $k_0 \neq 0$. Then the essential spectrum covers the whole line, that is, $\sigma_{\text{ess}}(\mathbb{H}) = \mathbf{R}$.*

Theorem 4.6 *Let $k_0 \neq 0$. Then \mathbb{H} has no eigenvalues, that is, $\sigma_{\text{p}}(\mathbb{H}) = \emptyset$.*

5 The canonical form of H_{DC} on the anti-symmetric space

We return to the familiar notation \mathbf{x}_j instead of \mathbf{r}_j . We may represent H_{DC} as follows. Recall

$$h_1 = (\vec{\sigma} \cdot \vec{p}_1) \otimes I_2, \quad h_2 = I_2 \otimes (\vec{\sigma} \cdot \vec{p}_2). \quad (5.1)$$

$$H_{DC}\Psi = \begin{pmatrix} (2m+V)I_4 & h_2 & h_1 & 0 \\ h_2 & VI_4 & 0 & h_1 \\ h_1 & 0 & VI_4 & h_2 \\ 0 & h_1 & h_2 & -(2m-V)I_4 \end{pmatrix} \begin{pmatrix} \vec{\psi}_{11}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{12}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{21}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{22}(\mathbf{x}_1, \mathbf{x}_2) \end{pmatrix}, \quad (5.2)$$

$$V(\mathbf{x}_1, \mathbf{x}_2) = V(\mathbf{x}_1) + V(\mathbf{x}_2) + V_0(\mathbf{x}_1, \mathbf{x}_2). \quad (5.3)$$

Proposition 5.1 *Let $\Psi \in \mathcal{H}^{\otimes 2} = L^2(\mathbf{R}^6; M(2, \mathbf{C}))^4$. Then*

$$H_{DC}\Psi = \begin{pmatrix} (2m+V)I_4 & (h)_2 & (h)_1 & 0 \\ (h)_2 & VI_4 & 0 & (h)_1 \\ (h)_1 & 0 & VI_4 & (h)_2 \\ 0 & (h)_1 & (h)_2 & -(2m-V)I_4 \end{pmatrix} \begin{pmatrix} \psi_{11}(\mathbf{x}_1, \mathbf{x}_2) \\ \psi_{12}(\mathbf{x}_1, \mathbf{x}_2) \\ \psi_{21}(\mathbf{x}_1, \mathbf{x}_2) \\ \psi_{22}(\mathbf{x}_1, \mathbf{x}_2) \end{pmatrix}, \quad (5.4)$$

where

$$(h)_1 \psi_{ij}(\mathbf{x}_1, \mathbf{x}_2) = \text{Mat} \left[((\vec{\sigma} \cdot \vec{p}_1) \otimes I_2) \vec{\psi}_{ij}(\mathbf{x}_1, \mathbf{x}_2) \right] = \vec{p}_1 \psi_{ij}(\mathbf{x}_1, \mathbf{x}_2) \cdot {}^t \vec{\sigma}, \quad (5.5)$$

$$(h)_2 \psi_{ij}(\mathbf{x}_1, \mathbf{x}_2) = \text{Mat} \left[(I_2 \otimes \vec{\sigma} \cdot \vec{p}_2) \vec{\psi}_{ij}(\mathbf{x}_1, \mathbf{x}_2) \right] = \vec{p}_2 \cdot \vec{\sigma} \psi_{ij}(\mathbf{x}_1, \mathbf{x}_2). \quad (5.6)$$

Proof: Let

$$\text{vec} \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a \\ c \\ b \\ d \end{pmatrix}. \quad (5.7)$$

Since

$$\text{Mat}[(A \otimes I_2) \text{vec} M] = M {}^t A, \quad \text{Mat}[(I_2 \otimes B) \text{vec} M] = BM \quad (5.8)$$

for any 2×2 matrices A and $M = (\Psi_k \otimes \Psi'_\ell)$, we arrive at the conclusion. Q.E.D.

Proposition 5.2 \mathcal{H}_A^2 is an invariant subspace of $\mathcal{H}^{\otimes 2} = \mathcal{H} \otimes \mathcal{H}$ with respect to the operator H_{DC} .

Proof: If $\psi_{12}(\mathbf{x}_2, \mathbf{x}_1) = -({}^t\psi_{21})(\mathbf{x}_1, \mathbf{x}_2)$, then $(\vec{p}_2\psi_{12})(\mathbf{x}_2, \mathbf{x}_1) = -(\vec{p}_1{}^t\psi_{21})(\mathbf{x}_1, \mathbf{x}_2)$. We shall check the first component of $H_{DC}\Psi$. In view of (5.5) and we find

$$\begin{aligned}
((h)_2\psi_{12} + (h)_1\psi_{21})(\mathbf{x}_2, \mathbf{x}_1) &= \vec{\sigma} \cdot \vec{p}_2\psi_{12}(\mathbf{x}_2, \mathbf{x}_1) + \sum_{j=1}^3 p_{1,j}\psi_{21}(\mathbf{x}_2, \mathbf{x}_1)({}^t\sigma_j) \\
&= -\vec{\sigma} \cdot \vec{p}_1({}^t\psi_{21})(\mathbf{x}_1, \mathbf{x}_2) - \sum_{j=1}^3 p_{2,j}({}^t\psi_{12})(\mathbf{x}_1, \mathbf{x}_2)({}^t\sigma_j) \\
&= -{}^t((h)_1\psi_{21})(\mathbf{x}_1, \mathbf{x}_2) - {}^t((h)_2\psi_{12})(\mathbf{x}_1, \mathbf{x}_2) \\
&= -{}^t((h)_2\psi_{12} + (h)_1\psi_{21})(\mathbf{x}_1, \mathbf{x}_2).
\end{aligned} \tag{5.9}$$

As for the second component, we see

$$\begin{aligned}
((h)_2\psi_{11} + (h)_1\psi_{22})(\mathbf{x}_2, \mathbf{x}_1) &= \vec{\sigma} \cdot \vec{p}_2\psi_{11}(\mathbf{x}_2, \mathbf{x}_1) + \sum_{j=1}^3 p_{1,j}\psi_{22}(\mathbf{x}_2, \mathbf{x}_1)({}^t\sigma_j) \\
&= -\vec{\sigma} \cdot \vec{p}_1({}^t\psi_{11})(\mathbf{x}_1, \mathbf{x}_2) - \sum_{j=1}^3 p_{2,j}({}^t\psi_{22})(\mathbf{x}_1, \mathbf{x}_2)({}^t\sigma_j) \\
&= -{}^t((h)_1\psi_{11})(\mathbf{x}_1, \mathbf{x}_2) - {}^t((h)_2\psi_{22})(\mathbf{x}_1, \mathbf{x}_2) \\
&= -{}^t((h)_2\psi_{11} + (h)_1\psi_{22})(\mathbf{x}_1, \mathbf{x}_2).
\end{aligned} \tag{5.10}$$

As for the third and fourth components, similar computations yield

$$((h)_1\psi_{11} + (h)_2\psi_{22})(\mathbf{x}_2, \mathbf{x}_1) = -{}^t((h)_1\psi_{11} + (h)_2\psi_{22})(\mathbf{x}_1, \mathbf{x}_2) \tag{5.11}$$

and

$$((h)_1\psi_{12} + (h)_2\psi_{21})(\mathbf{x}_2, \mathbf{x}_1) = -{}^t((h)_1\psi_{12} + (h)_2\psi_{21})(\mathbf{x}_1, \mathbf{x}_2). \tag{5.12}$$

Q.E.D.

The anti-symmetric property implies the following identities.

Lemma 5.3 Suppose that $F, G \in \mathcal{H}_A^2$. Then for any quadruple of indices i, j, k, ℓ ,

$$\langle (\vec{\sigma} \cdot \vec{p}_\tau \otimes I_2) \vec{F}_{ij}, \vec{G}_{k\ell} \rangle = \langle (I_2 \otimes \vec{\sigma} \cdot \vec{p}_\tau) \vec{F}_{ji}, \vec{G}_{\ell k} \rangle, \text{ for } \tau = 1, 2, \tag{5.13}$$

$$\langle V \vec{F}_{ij}, \vec{G}_{ij} \rangle = \langle V \vec{F}_{ji}, \vec{G}_{ji} \rangle \tag{5.14}$$

if V is a diagonal matrix satisfying

$$V(\mathbf{x}_1, \mathbf{x}_2) = V(\mathbf{x}_2, \mathbf{x}_1). \tag{5.15}$$

Proof: For simplicity, we only consider the case when $\tau = 2$. Both $\psi \in \mathcal{H}_S^2$ and $\varphi \in \mathcal{H}_A^2$ satisfy

$$\begin{aligned}
\partial_{\mathbf{x}_2} \vec{\psi}_{ij}(\mathbf{x}_1, \mathbf{x}_2) &= \text{vec}[\partial_{\mathbf{x}_1} {}^t\psi_{ji}](\mathbf{x}_2, \mathbf{x}_1), \\
\partial_{\mathbf{x}_2} \vec{\varphi}_{ij}(\mathbf{x}_1, \mathbf{x}_2) &= -\text{vec}[\partial_{\mathbf{x}_1} {}^t\varphi_{ji}](\mathbf{x}_2, \mathbf{x}_1).
\end{aligned} \tag{5.16}$$

for any $i, j = 1, 2$.

Hence for any $\psi, \varphi \in \mathcal{H}_S^2$,

$$\begin{aligned}
& \langle I_2 \otimes \vec{\sigma} \cdot \nabla_{\mathbf{x}_2} \vec{\psi}_{ij}, \vec{\varphi}_{kl} \rangle \\
&= \int_{\mathbf{R}^6} \text{tr}((\vec{\sigma} \cdot \nabla_{\mathbf{x}_2} \psi_{ij})(\mathbf{x}_1, \mathbf{x}_2) {}^t \overline{\varphi}_{kl}(\mathbf{x}_1, \mathbf{x}_2)) d\mathbf{x}_1 d\mathbf{x}_2 \\
&= \int_{\mathbf{R}^6} \text{tr}(\vec{\sigma} \cdot \nabla_{\mathbf{x}_1} {}^t \psi_{ji}(\mathbf{x}_2, \mathbf{x}_1) \overline{\varphi}_{lk}(\mathbf{x}_2, \mathbf{x}_1)) d\mathbf{x}_1 d\mathbf{x}_2 \\
&= \int_{\mathbf{R}^6} \text{tr}((\nabla_{\mathbf{x}_1} \psi_{ji}(\mathbf{x}_2, \mathbf{x}_1) \cdot {}^t \sigma) {}^t \overline{\varphi}_{lk}(\mathbf{x}_2, \mathbf{x}_1)) d\mathbf{x}_2 d\mathbf{x}_1 \\
&= \langle \vec{\sigma} \cdot \nabla_{\mathbf{x}_2} \otimes I_2 \vec{\psi}_{ji}, \vec{\varphi}_{lk} \rangle.
\end{aligned} \tag{5.17}$$

Here, we have used

$$\text{tr}(AB) = \text{tr}({}^t(AB)) = \text{tr}({}^tB {}^tA) = \text{tr}({}^tA {}^tB). \tag{5.18}$$

Similarly, we see that for any $\psi, \varphi \in \mathcal{H}_A^2$,

$$\langle I_2 \otimes \vec{\sigma} \cdot \nabla_{\mathbf{x}_2} \vec{\psi}_{ij}, \vec{\varphi}_{kl} \rangle = \langle \vec{\sigma} \cdot \nabla_{\mathbf{x}_2} \otimes I_2 \vec{\psi}_{ji}, \vec{\varphi}_{lk} \rangle. \tag{5.19}$$

Q.E.D.

Theorem 5.4 *Let*

$$H_{DC}^+ \Psi = \begin{pmatrix} V+2m & h_{12} & 0 & 0 \\ h_{12} & V & 0 & 0 \\ 0 & 0 & V & h_{12} \\ 0 & 0 & h_{12} & V-2m \end{pmatrix} \begin{pmatrix} \vec{\psi}_{11}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{12}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{21}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{22}(\mathbf{x}_1, \mathbf{x}_2) \end{pmatrix} \tag{5.20}$$

and

$$H_{DC}^- \Psi = \begin{pmatrix} V+2m & 0 & h_{21} & 0 \\ 0 & V & 0 & h_{21} \\ h_{21} & 0 & V & 0 \\ 0 & h_{21} & 0 & V-2m \end{pmatrix} \begin{pmatrix} \vec{\psi}_{11}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{12}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{21}(\mathbf{x}_1, \mathbf{x}_2) \\ \vec{\psi}_{22}(\mathbf{x}_1, \mathbf{x}_2) \end{pmatrix}, \tag{5.21}$$

where

$$\begin{aligned}
h_{12} &= I_2 \otimes (\vec{\sigma} \cdot \vec{p}_1) + I_2 \otimes (\vec{\sigma} \cdot \vec{p}_2). \\
h_{21} &= (\vec{\sigma} \cdot \vec{p}_1) \otimes I_2 + (\vec{\sigma} \cdot \vec{p}_2) \otimes I_2.
\end{aligned}$$

Then, If $\Psi, \Phi \in \mathcal{H}_A^2 \cap C_0^\infty$, then

$$\langle H_{DC} \Psi, \Phi \rangle = \langle H_{DC}^+ \Psi, \Phi \rangle, \quad \langle H_{DC} \Psi, \Phi \rangle = \langle H_{DC}^- \Psi, \Phi \rangle. \tag{5.22}$$

Proof of Theorem 5.4 We need to consider both (5.1) and their variants as follows.

$$\check{h}_1 = I_2 \otimes (\vec{\sigma} \cdot \vec{p}_1), \quad \check{h}_2 = (\vec{\sigma} \cdot \vec{p}_2) \otimes I_2.$$

By virtue of Lemma 5.3, we have

$$\langle h_1 \vec{\psi}_{21}, \vec{\phi}_{11} \rangle = \langle \check{h}_1 \vec{\psi}_{12}, \vec{\phi}_{11} \rangle, \quad \langle h_1 \vec{\psi}_{12}, \vec{\phi}_{22} \rangle = \langle \check{h}_1 \vec{\psi}_{21}, \vec{\phi}_{22} \rangle, \quad (5.23)$$

$$\langle h_1 \vec{\psi}_{11}, \vec{\phi}_{21} \rangle = \langle \check{h}_1 \vec{\psi}_{11}, \vec{\phi}_{12} \rangle, \quad \langle h_1 \vec{\psi}_{22}, \vec{\phi}_{12} \rangle = \langle \check{h}_1 \vec{\psi}_{22}, \vec{\phi}_{21} \rangle, \quad (5.24)$$

which implies

$$\langle H_{DC} \Psi, \Phi \rangle = \langle H_{DC}^+ \Psi, \Phi \rangle. \quad (5.25)$$

Similarly,

$$\langle h_2 \vec{\psi}_{12}, \vec{\phi}_{11} \rangle = \langle \check{h}_2 \vec{\psi}_{21}, \vec{\phi}_{11} \rangle, \quad \langle h_2 \vec{\psi}_{21}, \vec{\phi}_{22} \rangle = \langle \check{h}_2 \vec{\psi}_{12}, \vec{\phi}_{22} \rangle,$$

$$\langle h_2 \vec{\psi}_{11}, \vec{\phi}_{12} \rangle = \langle \check{h}_2 \vec{\psi}_{11}, \vec{\phi}_{2} \rangle, \quad \langle h_2 \vec{\psi}_{22}, \vec{\phi}_{21} \rangle = \langle \check{h}_2 \vec{\psi}_{22}, \vec{\phi}_{1,2} \rangle,$$

which implies

$$\langle H_{DC} \Psi, \Phi \rangle = \langle H_{DC}^- \Psi, \Phi \rangle. \quad (5.26)$$

Q.E.D.

6 Proof of the spectral properties of H_{DC}

6.1 Essential selfadjointness

Proof of Theorem 4.1: In view of Theorem 5.4, we can identify H_{DC} with H_{DC}^+ .

Lemma 6.1 *Let $\varphi(t) \in C^\infty(\mathbf{R}) \cap L^\infty(\mathbf{R})$. Then*

$$[H_{DC}^+, \varphi(|\mathbf{x}_1 - \mathbf{x}_2|)] = 0. \quad (6.1)$$

Let $\chi \in C_0^\infty(\mathbf{R})$ satisfy that $0 \leq \chi \leq 1$,

$$\chi(t) = \begin{cases} 1, & t \geq 2, \\ 0, & t \leq 1, \end{cases} \quad (6.2)$$

and B_n be a multiplication operator defined by $B_n = \chi(n|\mathbf{x}_1 - \mathbf{x}_2|)$ and

$$V_n = B_n V B_n. \quad (6.3)$$

Lemma 6.2 $H_{DC,n} = H_{DC,0} + V_n$ is essentially selfadjoint on $[C_0^\infty(\mathbf{R}^3; \mathbf{C}^4)]^{\otimes 2} \cap \mathcal{H}_A^2$.

Lemma 6.3

$$\lim_{n \rightarrow \infty} (H^* B_n \psi, \psi - B_n \psi) = 0 \quad (6.4)$$

for any $\psi \in D(H^*)$.

Thanks to Theorem 5.2 of Thaller [12], from Lemma 6.2 and Lemma 6.3, it follows that H_{DC} is also essentially selfadjoint on $[C_0^\infty(\mathbf{R}^3; \mathbf{C}^4)]^{\otimes 2} \cap \mathcal{H}_A^2$.

Now we are in a position to prove Lemma 6.2. We consider an orthogonal transformation S in $M(8, \mathbf{C})$

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} I_4 & I_4 \\ I_4 & -I_4 \end{pmatrix}. \quad (6.5)$$

Then

$$S^{-1} \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} S = \frac{1}{2} \begin{pmatrix} a+b & a-b \\ a-b & a+b \end{pmatrix}, \quad (6.6)$$

$$S^{-1} \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix} S = \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix}. \quad (6.7)$$

With the orthogonal transformation

$$T = S \oplus S \quad (6.8)$$

we therefore have

$$\begin{aligned} & T^{-1} H_{DC,n} T \\ &= \begin{pmatrix} h_{12} + V_n + m & m & 0 & 0 \\ m & -h_{12} + V_n + m & 0 & 0 \\ 0 & 0 & h_{12} + V_n - m & -m \\ 0 & 0 & -m & -h_{12} + V_n - m \end{pmatrix} \end{aligned} \quad (6.9)$$

$$= \begin{pmatrix} H_{00} & 0 & 0 & 0 \\ 0 & -H_{00} & 0 & 0 \\ 0 & 0 & H_{00} & 0 \\ 0 & 0 & 0 & -H_{00} \end{pmatrix} + m \begin{pmatrix} I_4 & I_4 & 0 & 0 \\ I_4 & I_4 & 0 & 0 \\ 0 & 0 & -I_4 & -I_4 \\ 0 & 0 & -I_4 & -I_4 \end{pmatrix} + V_n I_{16}, \quad (6.10)$$

where

$$H_{00} = h_{12} = I_2 \otimes [\vec{\sigma} \cdot (\vec{p}_1 + \vec{p}_2)]. \quad (6.11)$$

Introducing a change of coordinates

$$\frac{1}{\sqrt{2}}(\mathbf{x}_1 + \mathbf{x}_2) = \mathbf{y}_1, \quad \frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2) = \mathbf{y}_2,$$

we find

$$H_{00} = \sqrt{2}[I_2 \otimes (\vec{\sigma} \cdot \vec{p}_{\mathbf{y}_1})], \quad (6.12)$$

$$V = \frac{\sqrt{2}k}{|\mathbf{y}_1 + \mathbf{y}_2|} + \frac{\sqrt{2}k}{|\mathbf{y}_1 - \mathbf{y}_2|} + \frac{k_0}{\sqrt{2}|\mathbf{y}_2|}. \quad (6.13)$$

Let $\mathbf{y}_1 = (\eta_1, \eta_2, \eta_3)$, $\vec{p} = (p_1, p_2, p_3)$ with $p_j = -i\partial_{\eta_j}$ and $\vec{\sigma} \cdot \vec{p} = \sum_{j=1}^3 \sigma_j p_j$, then it holds that

$$H_{00}^2 = 2(I_2 \otimes (\vec{\sigma} \cdot \vec{p}))^2 = 2|\vec{p}|^2 I_4. \quad (6.14)$$

We note that H_{00} satisfies similar estimates to the ones for the Dirac operator $\vec{\alpha} \cdot \vec{p}$ (see [8], [9]).

Lemma 6.4

$$\| |\mathbf{y}_1|^{1/2} H_{00} u \|_{L^2(\mathbf{R}^6)^4} \geq \| |\mathbf{y}_1|^{-1/2} u \|_{L^2(\mathbf{R}^6)^4} \quad (6.15)$$

provided that u and $\nabla_{\mathbf{y}_1} u \in L^2(\mathbf{R}^6; \mathbf{C}^4)$.

Lemma 6.5 Let $Q \in L_{\text{loc}}^\infty(\mathbf{R}^3 \setminus \{0\})^{4 \times 4}$ be an Hermitian matrix which commutes with $I_2 \otimes (\vec{\sigma} \cdot \vec{\mathbf{y}}_1)$ ($\vec{\mathbf{y}}_1 \in \mathbf{R}^3$), and which satisfies

$$|Q(\mathbf{y}_1)| \leq \sqrt{2}\mu |\mathbf{y}_1|^{-1}, \quad 0 \leq \mu < \sqrt{3}/2. \quad (6.16)$$

Then for all $v \in H^1(\mathbf{R}^6; \mathbf{C}^4)$ we have

$$\| \sqrt{2} |\mathbf{y}_1|^{-1} v \|_{L^2(\mathbf{R}^6)^4} \leq \frac{1}{1-a} \| (H_{00} + Q(\mathbf{y}_1)) v \|_{L^2(\mathbf{R}^6)^4}, \quad a = \sqrt{\mu^2 + 1/4}. \quad (6.17)$$

These inequalities can be proved by introducing polar coordinates in the variable \mathbf{y}_1 just as in the case of the usual Dirac operator (Schmincke [8,9]).

Without loss of generality, we may assume that $m = 0$.

Proposition 6.6 Suppose that $|k| < \sqrt{3}/2$ and $k_0 \neq 0$. Then, $H_n := H_{00} + V_n$ is essentially self-adjoint on $C_0^\infty(\mathbf{R}^6; \mathbf{C}^4)$.

Proof: It suffices to show that

$$\overline{(H_n \pm iI_4)(C_0^\infty(\mathbf{R}^6; \mathbf{C}^4))} = L^2(\mathbf{R}^6; \mathbf{C}^4). \quad (6.18)$$

Due to the cutoff function, the scalar potential V_n has singularities which do not coincide, so that we are able to employ a technique similar to the one developed by Vogelsang ([13]) in view of the following lemma which can be shown to be based on Lemma 6.4. Q.E.D.

Proof of Lemma 6.2 From Proposition 6.6, it follows that

$$\overline{(H_{DC,n} \pm iI_4)([C_0^\infty(\mathbf{R}^6; \mathbf{C}^4)]^{\otimes 2})} = L^2(\mathbf{R}^6; \mathbf{C}^{16}). \quad (6.19)$$

Since $[C_0^\infty(\mathbf{R}^3; \mathbf{C}^4)]^{\otimes 2} \cap \mathcal{H}_A^2$ is an invariant subspace of $H_{DC,n}$, we can conclude that $H_{DC,n}$ is essentially selfadjoint in $\mathcal{H}_A^{\otimes 2}$. Q.E.D.

6.2 Essential spectrum

Proof of Theorem 4.2 Let $\lambda > m$, $\mu > m$. Take $\xi, \eta \in \mathbf{R}^3 \setminus \{0\}$ such that

$$|\xi|^2 + m^2 = \lambda^2, \quad |\eta|^2 + m^2 = \mu^2, \quad \xi \cdot \eta = 0. \quad (6.20)$$

For each $\xi \in \mathbf{R}^3$, let $u, v \in \mathbf{C}^4 \setminus \{0\}$ be normalized eigenvectors to the equations

$$(\alpha \cdot \xi + m\beta)u = \lambda u, \quad |u|_{\mathbf{C}^4} = 1, \quad (6.21)$$

$$(\alpha \cdot \xi + m\beta)v = -\mu v, \quad |v|_{\mathbf{C}^4} = 1, \quad (6.22)$$

respectively. Define two functions by

$$u_n(\mathbf{x}) = \chi_n(\mathbf{x}) e^{i\mathbf{x} \cdot \xi} u(\xi), \quad v_n(\mathbf{x}) = \chi_n(\mathbf{x}) e^{i\mathbf{x} \cdot \eta} v(\eta), \quad (6.23)$$

where $\chi_n \in C_0^\infty(\mathbf{R}^3)$ is a nonnegative function such that

$$\int_{\mathbf{R}^3} |\chi_n(\mathbf{x})|^2 d\mathbf{x} = 1, \quad \text{supp}\chi_n \subset \{\mathbf{x} \in \mathbf{R}^3 \mid n < |\mathbf{x}| < 2n\}. \quad (6.24)$$

Then $\{u_n(\mathbf{x})\}$ and $\{v_n(\mathbf{x})\}$ are two sets of singular sequences in $L^2(\mathbf{R}^3)^4$ such that

$$\|u_n\|_{L^2} = \|v_n\|_{L^2} = 1, \quad u_n \rightharpoonup 0, \quad v_n \rightharpoonup 0, \quad \text{weakly}, \quad (6.25)$$

$$[H_0 + m\beta - \lambda]u_n \longrightarrow 0 \quad (n \rightarrow \infty), \quad \text{supp}u_n \subset \{\mathbf{x} \in \mathbf{R}^3 \mid n < |\mathbf{x}| < 2n\} \quad (6.26)$$

$$[H_0 + m\beta + \mu]v_n \longrightarrow 0 \quad (n \rightarrow \infty), \quad \text{supp}v_n \subset \{\mathbf{x} \in \mathbf{R}^3 \mid n < |\mathbf{x}| < 2n\}. \quad (6.27)$$

Now we shall construct a singular sequence in \mathcal{H}_A^2 .

Lemma 6.7

$$w_n := \frac{1}{\sqrt{2}}\{u_{n^2} \otimes v_n - v_n \otimes u_{n^2}\} \in \mathcal{H}_A^2, \quad (6.28)$$

Proof: Let us consider $F = f_1 \otimes \mathbf{i} + f_2 \otimes \mathbf{j}$, $G = g_1 \otimes \mathbf{i} + g_2 \otimes \mathbf{j} \in L^2(\mathbf{R}^3)^4$, where $f_j, g_j \in L^2(\mathbf{R}^3)^2$. Recall the definition of $u \otimes v$:

$$F \otimes G = (f_1 \otimes g_1) \otimes (\mathbf{i} \otimes \mathbf{i}) + (f_1 \otimes g_2) \otimes (\mathbf{i} \otimes \mathbf{j}) + (f_2 \otimes g_1) \otimes (\mathbf{j} \otimes \mathbf{i}) + (f_2 \otimes g_2) \otimes (\mathbf{j} \otimes \mathbf{j}), \quad (6.29)$$

where $f_j \otimes g_k$ ($j, k = 1, 2$) are defined as

$$f_j \otimes g_k = \begin{pmatrix} u_{1,j} \otimes v_{1,k} \\ u_{1,j} \otimes v_{2,k} \\ u_{2,j} \otimes v_{1,k} \\ u_{2,j} \otimes v_{2,k} \end{pmatrix} = \begin{pmatrix} u_{1,j}(\mathbf{x}_1)v_{1,k}(\mathbf{x}_2) \\ u_{1,j}(\mathbf{x}_1)v_{2,k}(\mathbf{x}_2) \\ u_{2,j}(\mathbf{x}_1)v_{1,k}(\mathbf{x}_2) \\ u_{2,j}(\mathbf{x}_1)v_{2,k}(\mathbf{x}_2) \end{pmatrix}. \quad (6.30)$$

for $f_j = \begin{pmatrix} u_{1,j} \\ u_{2,j} \end{pmatrix}$ and $g_k = \begin{pmatrix} v_{1,k} \\ v_{2,k} \end{pmatrix}$.

It follows that

$$\begin{aligned} F \otimes G - G \otimes F &= (f_1 \otimes g_1 - g_1 \otimes f_1) \otimes (\mathbf{i} \otimes \mathbf{i}) + (f_1 \otimes g_2 - g_1 \otimes f_2) \otimes (\mathbf{i} \otimes \mathbf{j}) \\ &\quad + (f_2 \otimes g_1 - g_2 \otimes f_1) \otimes (\mathbf{j} \otimes \mathbf{i}) + (f_2 \otimes g_2 - g_2 \otimes f_2) \otimes (\mathbf{j} \otimes \mathbf{j}) \\ &\in \mathcal{H}_A^2. \end{aligned} \quad (6.31)$$

Q.E.D.

From Lemma 6.7, it follows that $\{w_n\}$ becomes a singular sequence of $H_{DC} - \lambda + \mu$. In fact, it satisfies that as $n \rightarrow \infty$

$$(H_{DC} - (\lambda - \mu))w_n = \frac{k}{|\mathbf{x}_1|}w_n + \frac{k}{|\mathbf{x}_2|}w_n + \frac{k_0}{|\mathbf{x}_1 - \mathbf{x}_2|}w_n \longrightarrow 0, \quad (6.32)$$

$$w_n \rightharpoonup 0, \quad \|w_n\|_{L^2} = 1. \quad (6.33)$$

The last assertion $\|w_n\|_{L^2} = 1$ follows from the fact that the eigenvectors $u(\xi)$, $v(\xi)$ corresponding to the different eigenvalues are orthogonal to each other. Since

$$(m, \infty) + (-\infty, -m) = (-\infty, \infty),$$

we can conclude that $\sigma_{\text{ess}}(H_{DC}) = \mathbf{R}$.

Q.E.D.

6.3 Absence of eigenvalues

Proof of Theorem 4.3 We first consider the case where $m > 0$.

Let $u \in \mathcal{H}_A^2$ be a solution to

$$H_{DC}u = \lambda u. \quad (6.34)$$

Then we see that for any function $\varphi(\mathbf{y}_1, \mathbf{y}_2) \in C_0^\infty(\mathbf{R}^6; \mathbf{C}^{16}) \cap \mathcal{H}_A^2$,

$$\langle H_{DC}u, \varphi \rangle_{\mathcal{H}_A^2} = \langle H_{DC}^+u, \varphi \rangle_{\mathcal{H}_A^2}. \quad (6.35)$$

Let

$$(Fu)(\mathbf{y}) = u((\mathbf{y}_1 + \mathbf{y}_2)/\sqrt{2}, (\mathbf{y}_1 - \mathbf{y}_2)/\sqrt{2}).$$

Then we see that for $v \in C_0^\infty(\mathbf{R}^6; \mathbf{C}^{16}) \cap \mathcal{H}_A^2$,

$$\langle H_{DC}Fu, Fv \rangle_{\mathcal{H}_A^2} = \langle H_{DC}^+Fu, Fv \rangle_{\mathcal{H}_A^2}, \quad (6.36)$$

so that we can identify H_{DC} with H_{DC}^+ in \mathcal{H}_A^2 . In view of (6.34), we have

$$H_{\mathbf{y}_2}(Fu)(\cdot, \mathbf{y}_2) = \left(\lambda - \frac{k_0}{\sqrt{2}|\mathbf{y}_2|} \right) (Fu)(\cdot, \mathbf{y}_2), \quad (6.37)$$

where $H_{\mathbf{y}_2}$ in $L^2(\mathbf{R}^3)^{16}$ is an operator with a parameter \mathbf{y}_2 defined by

$$H_{\mathbf{y}_2} = \begin{pmatrix} H_{00} + mI_4 & mI_4 & 0 & 0 \\ mI_4 & -H_{00} + mI_4 & 0 & 0 \\ 0 & 0 & H_{00} - mI_4 & -mI_4 \\ 0 & 0 & -mI_4 & -H_{00} - mI_4 \end{pmatrix} + V_{\mathbf{y}_2}I_{16}, \quad (6.38)$$

with

$$V_{\mathbf{y}_2} = \frac{\sqrt{2}k}{|\mathbf{y}_1 + \mathbf{y}_2|} + \frac{\sqrt{2}k}{|\mathbf{y}_1 - \mathbf{y}_2|}. \quad (6.39)$$

Let

$$H_{++} = \begin{pmatrix} H_{00} + mI_4 & mI_4 \\ mI_4 & -H_{00} + mI_4 \end{pmatrix}, \quad H_{--} = \begin{pmatrix} H_{00} - mI_4 & -mI_4 \\ -mI_4 & -H_{00} - mI_4 \end{pmatrix}. \quad (6.40)$$

Then,

$$(H_{++} - mI_8)^2 = (|p|^2 + m^2)I_8, \quad (H_{--} + mI_8)^2 = (|p|^2 + m^2)I_8 \quad (6.41)$$

with $p = -i\nabla_{\mathbf{y}_1}$. Since

$$\sigma_{ess}(H_{++} - mI_8) = (-\infty, -m] \cup [m, \infty), \quad (6.42)$$

$$\sigma_{ess}(H_{--} + mI_8) = (-\infty, -m] \cup [m, \infty) \quad (6.43)$$

and $\lim_{|\mathbf{y}_1| \rightarrow \infty} V_{\mathbf{y}_2} = 0$, it holds that

$$\sigma_{ess}(H_{++} + V_{\mathbf{y}_2} I_4) = (-\infty, 0] \cup [2m, \infty), \quad (6.44)$$

$$\sigma_{ess}(H_{--} + V_{\mathbf{y}_2} I_4) = (-\infty, -2m] \cup [0, \infty). \quad (6.45)$$

On the other hand, because of Theorem 4.1, a technique of Weidmann ([14] Theorem 10.38) and Kalf [3] enables us to prove that $H_{\pm\pm} + V_{\mathbf{y}_2} I_4$ have no eigenvalues in $(-\infty, 0] \cup [2m, \infty)$ and $(-\infty, -2m] \cup [0, \infty)$, respectively. Therefore, we see that every eigenvalue of $H_{\mathbf{y}_2}$ is in $(-2m, 0) \cup (0, 2m)$ and its multiplicity is finite if it exists.

For any fixed $\mathbf{y}_2 \in \mathbf{R}^3 \setminus \{0\}$ and $\kappa > 0$, define an operator in $L^2(\mathbf{R}^3)^{16}$

$$H(\kappa) = H_{\kappa \mathbf{y}_2}.$$

The family of operators $\{H(\kappa)\}_{\kappa > 0}$ forms an analytic family of type (A) with a common domain \mathcal{D}

$$\mathcal{D} = \{u \in L^2(\mathbf{R}^3)^{16} \mid \nabla_{\mathbf{y}_1} u \in L^2(\mathbf{R}^3)^{16}\}.$$

Therefore, we note that each eigenvalue $E_n(\kappa)$ of $H(\kappa)$ is an analytic function of $\kappa > 0$. Now we claim

Lemma 6.8 *Let $u \in \mathcal{H}_A^2$ be a solution to the equation (6.34). Then $u = 0$ almost everywhere in \mathbf{R}^6 .*

Proof: We assume that u is nonzero vector in an open subset Γ with positive measure. Then it holds that there exists a nonempty open ball B_0 in \mathbf{R}^3 such that for all $\mathbf{y}_2 \in B_0$,

$$\|Fu(\cdot, \mathbf{y}_2)\|_{L^2(\mathbf{R}^3)^{16}} \neq 0. \quad (6.46)$$

Fix $\mathbf{y}_2 \in B_0$. Then in view of (6.37), it holds that for some n and every κ near 1

$$E_n(\kappa) = \lambda - k_0/|\kappa \mathbf{y}_2|. \quad (6.47)$$

From the analyticity it follows that for any $\kappa > 0$

$$\lambda - k_0/|\sqrt{2}\kappa \mathbf{y}_2| = E_n(\kappa), \quad (6.48)$$

which contradicts the fact that $E_n(\kappa) \in (-2m, 0) \cup (0, 2m)$ and $k_0 \neq 0$. Q.E.D.

When $m = 0$, we see that for any $\kappa > 0$, $H(\kappa)$ has no eigenvalues in $(-\infty, 0) \cup (0, \infty)$, so that we would have

$$0 = \lambda - \frac{k_0}{|\kappa \mathbf{y}_2|} \quad (6.49)$$

if eigenvalues existed. It leads to a contradiction.

Q.E.D.

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